Verification of the MC²-3 Gamma Library

Nuclear Science and Engineering Division

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September 30, 2018

ABSTRACT

The new gamma library was generated based on the 94-group gamma structure, including delayed gamma and beta data, using the PreGAMMA and GenGAMMA codes with ENDF/B-VII.0 data. The new gamma library was first verified using the 2D benchmark problems that were introduced in the GAMSOR manual, showing that the neutron and gamma heatings from DIF3D were in good agreement with MCNP solutions within 5% even in the non-fuel regions of both cores with uranium or plutonium dominant fuel compositions. Similarly, the DIF3D power solutions for additional simpler 1D problems with 3 or 6 regions showed good agreement with MCNP solutions. Note that all DIF3D calculations were based on the 230-group neutron and 94-group gamma data.

For the EBR-II benchmark problem, the DIF3D solution with the new gamma library maintained good agreement in the power distribution with the MCNP solution, which is comparable to the DIF3D results with the current 21-group gamma library. The use of delayed gamma and beta data increased powers at the dummy assemblies by 26%, which appears to be reasonable. Further detailed verification tests may be necessary and, more importantly, validation tests are required against measurement data.

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1. Introduction

A new gamma library has been generated based on the 94-group gamma structure, including delayed gamma and beta data and improving the current 21-group gamma library. Preliminary verification tests [1] for the new gamma library were performed using the ABTR fuel pin problem [2] and EBR-II benchmark problem [3], demonstrating that the DIF3D [4] solutions with the library were reasonable compared to those with the current 21-group gamma library and corresponding MCNP solutions. However, further thorough verification tests are needed to check the prompt gamma and heating data for individual isotopes and the delayed gamma and beta data that are newly included in the new library.

The new gamma library was generated using the PreGAMMA and GenGAMMA codes [1] using ENDF/B-VII.0 data. MC²-3 has been updated [5] to be able to process the new library: i.e., read the new library, generate PMATRX with the updated heating data, solve the gamma transport equations using the 94-group gamma cross sections, and condense the gamma cross sections to the 21-group data using the 94-group gamma flux solutions.

With the new gamma library, attempts were made to verify the neutron and gamma heating data for individual isotopes and to solve the EBR-II 138B benchmark problem again to confirm the previous calculation results and compare solution accuracies between the current and new libraries. In addition, the 2D benchmark problem discussed in the GAMSOR manual [6] was revisited since noticeable errors in gamma heatings in the non-fuel regions were reported in the document. For further investigation, simpler 1D benchmark problems were devised to compare neutron and gamma heating between MC²-3/DIF3D/GAMSOR and MCNP, in which no contribution of delayed gamma and betas were considered for the consistent comparison.

A brief introduction of neutron and gamma heating methodologies and the current status of the gamma libraries are presented in Section 2. Verification tests including the 2D benchmark problem and the EBR-II benchmark problem are described in details in Section 3. Conclusions are discussed in Section 4.

2. Generation of Gamma Libraries

The energy released from fission should be equal to the sum of the kinetic energy of the fission fragments and emitted neutrons (both prompt and delayed), the energy of both prompt and delayed γ and β radiations. The neutrinos and anti-neutrinos released during the fission process produce energy but due to the extremely low interaction probability these neutrinos and anti-neutrinos are assumed to get out of the system without depositing any energy in the system.

The total energy release from fission can be represented as

$$Q_f = Q_k + Q_{p,n} + Q_{p,\gamma} + Q_{d,n} + Q_{d,\gamma} + Q_{d,\beta} + Q_\nu, \quad (1)$$

where Q_k : the kinetics energy of the fission fragments,

$Q_{p,n}$: the kinetics energy of the prompt fission neutrons,

$Q_{p,\gamma}$: the kinetics energy of the prompt gamma rays,

$Q_{d,n}$: the kinetics energy of the delayed fission neutrons,

$Q_{d,\gamma}$: the kinetics energy of the delayed gamma rays,

$Q_{d,\beta}$: the energy of the delayed beta radiation,

Q_ν : the energy of the neutrinos.

The fission energy release components are dependent on the energy of the neutron that induced fission. Neutrinos do not deposit their energy in the system and thus recoverable energy does not include neutrinos.

Neutron KERMA

A KERMA (Kinetic Energy Release in Materials) factor is defined as an averaged kinetic energy release per reaction times a cross section [7]:

$$k_{ij}(E) = \sum_l \bar{E}_{ijl}(E) \sigma_{ij}(E), \quad (1)$$

where $\bar{E}_{ijl}$ is the total kinetic energy carried away by the l^{th} species of secondary particles, and σ_{ij} is the cross section for material i and reaction j . The KERMA factor is computed by the following energy-balance method:

$$k_{ij}(E) = (E + Q_{ij} - \bar{E}_{ijn} - \bar{E}_{ij\gamma}) \sigma_{ij}(E), \quad (2)$$

where E is the incident neutron energy, Q_{ij} is the reaction mass difference, and $\bar{E}_{ijn}$ and $\bar{E}_{ij\gamma}$ are the total energy of secondary neutron including multiplicity and that of photon including multiplicity, respectively. Eq. (2) assumes that all secondary particles except for neutrons and gammas deposit their energy locally. This assumption is not correct in some cases, however most other secondary particles which are massive deposit their energy locally. If the gamma energy is deposited locally, $\bar{E}_{ijr}$ is set to zero in the equation.

The neutron KERMA is calculated in the HEATR module of NJOY [7], which are treated as cross sections in the GROUPT module in NJOY. In the processing, a 1/E spectrum is normally specified for the entire group range with the infinite background cross section (infinite dilute). Therefore, an actual resonance self-shielding effect to KERMA factors is accounted for in the MC²-3 calculation.

Gamma KERMA

The gamma KERMA is defined similarly to the neutron KERMA. The energy dependent gamma KERMA factor for isotope is determined as

$$k_i(E) = E(\sigma_{i,pe}(E) + \sigma_{i,ca}(E)) + (E - 1.02\text{MeV})\sigma_{i,pp}(E), \quad (3)$$

where $\sigma_{i,pe}$, $\sigma_{i,ca}$, and $\sigma_{i,pp}$ are the photoelectric, Compton absorption, and pair production cross sections, respectively. All energy is deposited or transported by other photons. In particular, the Compton scattered photon's energy is transported elsewhere in the gamma flux calculation. The two 0.51 MeV photons (total 1.02 MeV) produced by the annihilation of the positron created in a pair production have their energy subtracted in the equation above.

The photoelectric absorption, Compton (incoherent) scattering, and pair production are dominant at low, intermediate (0.2–5 MeV), and high energies, respectively, due to their reaction characteristics. As the atomic number increase, the photoelectric effect becomes much more dominant and pair production becomes more dominant than Compton scattering because there are more atomic electrons to interact with which lead to a higher cross section.

A typical energy release from U-235 is shown in Table 2-1. The total recoverable energy from a fission event is about 193.7 MeV. The energies from fission fragment and delay betas are deposited locally and part of the other energies including prompt neutron and gamma and delayed gamma are transported to neighboring regions in the core. The total energy will include the energy produced from captured gammas shown in Figure 2-1.

Table 2-1. Energy Release in Fission

Quantity	MeV	Deposit Site
Kinetic energy of fission fragments	169.1	Local
Kinetic energy of prompt neutrons	4.79	Global
Kinetic energy of prompt gammas	6.97	Global
Kinetic energy of delayed gammas	6.33	Global
Total energy released by delayed betas	6.5	Local
Total recoverable energy	193.7	

The total reactor gammas consists of prompt and delayed gammas. Prompt gammas are produced at the fission event or by the radioactive capture reaction and the inelastic scattering reactions, while delayed gammas are generated from the decay of fission product and the decay of neutron activation products. Delayed betas are generated from activation and fission.

Figure 2-1. Isotopic Fission and Gamma Energy Deposited without Transport

The current version of the gamma library available in the /software/MCC3 directory was updated in 2016. Recently a new gamma library were generated to improve the accuracy of neutron and gamma heating calculations. The updates in the new gamma library are as follows:

- 1) The 94-group gamma group structure is used,
- 2) Some missing neutron heatings are included,
- 3) Delayed gamma and beta data included.

The gamma data including PMATRX and GAMISO are produced from MC²-3 together with the neutron cross sections for each region. For the gamma data, MC²-3 provides the following three options for users to generate them:

- 1) Generate the 21-group gamma data using the 21-group gamma library,
- 2) Generate the 21-group gamma data using the 94-group gamma library,
- 3) Generate the 94-group gamma data using the 94-group gamma library.

As indicated, the options 2 and 3 requires the 94-group gamma library. For the option 2, the group condensation from 94 to 21-group data should be involved using the spectra calculated for a homogeneous composition in MC²-3 itself or a RZ model based on the two-step approach with MC²-3/TWODANT. The latter involves a 94-group gamma transport calculation with TWODANT. In this verification work, we tried the options 1 and 3 to make the data processing process simple.

3. Verification Tests

3.1 Isotopic Gamma Heating

For clear verification tests of the new gamma library, three homogeneous compositions were selected as described in Table 3-1. In MC²-3, the neutron flux calculation was first performed for each composition, and the 94-group gamma sources were calculated using the neutron fluxes and gamma production matrices obtained from the gamma library. Then, the gamma transport calculation (slowing down for these cases) was conducted using the gamma interaction cross sections available from the gamma library.

Table 3-1. Homogeneous Compositions for Gamma Flux Calculation

Composition	Isotope			
1	U-235			
2	U-235	2.0000E-03	U-238	7.5000E-03
3	Cr-52	2.0173E-03	Zr-90	1.6788E-03
	Ni-58	6.7965E-05	Na-23	7.1453E-03
	Fe-56	1.4857E-02	U-235	1.2000E-03
	Mo-98	1.3316E-04	U-238	7.4400E-03
	Mn-55	1.0666E-04

Figure 3-1. Gamma Flux Distribution Before and After Gamma Transport Calculation for the Homogeneous Composition 1

Figure 3-2. Gamma Flux Distribution Before and After Gamma Transport Calculation for the Homogeneous Composition 2

Figure 3-3. Gamma Flux Distribution Before and After Gamma Transport Calculation for the Homogeneous Composition 3

Figure 3-1, Figure 3-2, and Figure 3-3 show the 230-group neutron fluxes and 94-group gamma fluxes before and after transport obtained from compositions 1, 2, and 3, respectively. Due to the slowing down of gamma photons in infinite media (the homogeneous compositions), the gamma fluxes after transport are shifted toward the lower energies compared to those before transport. In the gamma fluxes after transport, the flux peaks at 0.5 MeV and 0.875 MeV come from U-235 and Fe-56, respectively.

Attempts were made to verify the neutron and gamma heatings for all isotopes available in the gamma library, but we realized that it was not easy to separate out kinetics energies from fission fragments, prompt neutrons and gammas, and delayed gammas and betas for individual isotopes except for a few fissionable isotopes including U-235. Thus, as shown in Figure 3-4, a simple 1D problem with two regions was devised to add an isotope of interest to a region and compare the gamma heating results from the region between MC²-3/DIF3D and MCNP. The reflective boundary condition was applied to both ends. In this problem, the gamma fluxes at the region of interest are determined by the gammas generated from neutron interaction with isotopes at the region and transported from the gammas generated at the other region. Therefore, the accuracy of gamma production and transport is checked in the way. Figure 3-5 shows % differences of gamma heatings between the two codes, indicating that the differences are less than 10% except for several isotopes (H-1, Sn-125, Nd-146, Pm-148, Pa-233, U-233, and Am-243). Those isotopes with noticeable differences should be investigated.

Figure 3-4. 1D Two-region Problem Used for Verification of Isotopic Gamma Heating

Figure 3-5. % Differences of Isotopic Gamma Heatings between MC²-3/DIF3D and MCNP

3.2 Simple Benchmark Problems

Simple 2D and 1D problems were constructed based on fast reactor compositions to verify the gamma library and calculation using MC²-3/DIF3D/GAMSOR (hereafter DIF3D represents

DIF3D-VARIANT). For 2D problems [6], two configurations were set up based upon a simple 2D. One is a uranium dominated core region in the core region with the control rod inserted in the outer core region (case 1), as shown in Figure 3-6. The other repeats case 1 but uses a plutonium dominated fuel composition in the core region (case 2). The problem is composed of an inner core, outer core, blanket, reflector and shield regions as shown in Figure 3-6, and the control rod (red colored) is inserted in the asymmetric location (in terms of a quarter core) of the outer core region.

The compositions for the 2D problem case 1 are given in Table 3-2. Material compositions for the 2D problem consists of a standard homogeneous mixture for sodium cooled fast reactors with zirconium alloyed fuel. The fuel content in the core region was simplified consisting of two uranium isotopes, U-235 and U-238, for case 1. For case 2, however, the core region is composed of normal uranium and plutonium isotopes as well as higher actinides, as shown in Table 3-3.

Figure 3-6. Configuration of the Simple 2D Test Problem

The 2D problem was further simplified to a 1D geometry for more clear verification minimizing the source of errors due to the transport calculation. In the 1D problem case 1, as shown in Figure 3-7, the compositions of the 2D problem with the uranium dominated core remained the same. The boundary conditions are basically the same as the 2D problem, having the reflective boundary condition to the left side and the vacuum boundary condition to the right side. The 1D problem case 2 was made by removing boron and carbon from the control rod and shield regions. Two more 1D problems were created by further simplifying regions with fuel and non-fuel regions only and maintaining the same boundary conditions, as shown in Figure 3-8. The fuel regions are composed of U-235 and U-238 and the non-fuel region contains only O-16 for case 3 and only Fe-56 and Na-23 for case 4, as shown in Table 3-4.

Figure 3-7. 1D Slab Problem with 6 Regions

Figure 3-8. 1D Slab Problem with 3 Regions

Reference calculations were performed using MCNP tallying total, neutron, and gamma power generated from prompt neutron and gamma only as well as 33 or 230 group neutron fluxes and 21 or 94 group gamma fluxes from 18 regions with 10 cm thick: e.g. for the 2D problem case 1, 5 regions for the inner core, 3 regions for the outer core, 2 regions for the control rod, 2 regions for the blanket, 3 regions for the reflector, and 3 regions for the shield.

Deterministic calculations were performed using MC²-3/DIF3D/GAMSOR. For the neutron calculation, the 33 group structure were used at the beginning, but we noticed that the estimated eigenvalues were accurate enough but the errors in flux distributions were significant. As well known, TWODANT calculations with the two step approach were required to use the 33 group cross sections in DIF3D. So, finally, the 230-group cross sections were used without TWODANT calculations to simplify the calculation step even though the DIF3D calculation time increased significantly.

For all DIF3D calculations, the P7P5 transport and anisotropic scattering approximation was used. GAMSOR was used to calculate gamma sources based on the neutron fluxes calculated from DIF3D and PMATRX generated from MC²-3. With the gamma source calculated from GAMSOR, the gamma transport calculation was performed using DIF3D with P7P5 and then powers were calculated with the heats generated from neutrons and gammas.

For the gamma calculation, the new 21-group gamma library were used at the beginning since from preliminary calculations we observed no noticeable differences in the results from the 21-group and 94-group gamma libraries, but later on the 94-group gamma library was utilized as well to see any change of errors arising from the number of gamma groups.

The new gamma library includes delayed gamma and delayed beta contributions to heating. However, for the comparison between DIF3D and MCNP solutions, the delayed contributions to heating were excluded since the MCNP solutions do not include them. Note that all calculations used the ENDF/B-VII.0 data.

Table 3-2. Material Compositions for the 2D Test Problem 1

Isotope	Inner Core	Outer Core	Blanket	Reflector	Shield	Control Rod
CR-50	1.0461E-04	1.0461E-04	1.0461E-04	3.8036E-04	1.3720E-04	1.2112E-04
CR-52	2.0173E-03	2.0173E-03	2.0173E-03	7.3349E-03	2.6458E-03	2.3356E-03
CR-53	2.2874E-04	2.2874E-04	2.2874E-04	8.3172E-04	3.0001E-04	2.6484E-04
CR-54	5.6939E-05	5.6939E-05	5.6939E-05	2.0703E-04	7.4679E-05	6.5924E-05
NI-58	6.7965E-05	6.7965E-05	6.7965E-05	2.4712E-04	8.9140E-05	7.8689E-05
NI-60	2.6180E-05	2.6180E-05	2.6180E-05	9.5192E-05	3.4337E-05	3.0311E-05
NI-61	1.1380E-06	1.1380E-06	1.1380E-06	4.1379E-06	1.4926E-06	1.3176E-06
NI-62	3.6285E-06	3.6285E-06	3.6285E-06	1.3193E-05	4.7590E-06	4.2011E-06
NI-64	9.2407E-07	9.2407E-07	9.2407E-07	3.3600E-06	1.2120E-06	1.0699E-06
FE-54	9.4643E-04	9.4643E-04	9.4643E-04	3.4413E-03	1.2413E-03	1.0958E-03
FE-56	1.4857E-02	1.4857E-02	1.4857E-02	5.4021E-02	1.9486E-02	1.7201E-02
FE-57	3.4311E-04	3.4311E-04	3.4311E-04	1.2476E-03	4.5001E-04	3.9726E-04
FE-58	4.5662E-05	4.5662E-05	4.5662E-05	1.6603E-04	5.9889E-05	5.2867E-05
MO-92	8.1308E-05	8.1686E-05	8.1686E-05	6.1129E-05	2.2050E-05	1.9465E-05
MO-94	5.0810E-05	5.1047E-05	5.1047E-05	3.8200E-05	1.3779E-05	1.2164E-05
MO-95	8.7528E-05	8.7935E-05	8.7935E-05	6.5805E-05	2.3737E-05	2.0954E-05
MO-96	9.1822E-05	9.2249E-05	9.2249E-05	6.9034E-05	2.4901E-05	2.1982E-05
MO-97	5.2627E-05	5.2872E-05	5.2872E-05	3.9566E-05	1.4272E-05	1.2599E-05
MO-98	1.3316E-04	1.3378E-04	1.3378E-04	1.0012E-04	3.6113E-05	3.1879E-05
MO-100	5.3233E-05	5.3480E-05	5.3480E-05	4.0021E-05	1.4436E-05	1.2744E-05
MN-55	1.0666E-04	1.0666E-04	1.0666E-04	3.8782E-04	1.3989E-04	1.2349E-04
NA-23	7.1453E-03	7.1453E-03	7.1453E-03	3.4976E-03	3.4976E-03	8.1722E-03
ZR-90	1.6788E-03	1.6788E-03	1.6788E-03			
ZR-91	3.6610E-04	3.6610E-04	3.6610E-04			
ZR-92	5.5959E-04	5.5959E-04	5.5959E-04			
ZR-94	5.6709E-04	5.6709E-04	5.6709E-04			
ZR-96	9.1361E-05	9.1361E-05	9.1361E-05			
U-235	1.2000E-03	2.0000E-03	2.0000E-05			
U-238	7.4400E-03	7.4400E-03	7.4400E-03			
B-10					8.1942E-03	5.9987E-03
B-11					3.2983E-02	2.4145E-02
C-12					1.9432E-03	1.4225E-03

Table 3-3. Fuel Compositions of the Core Regions for the 2D Test Problem 2

Isotope	ND	Isotope	ND	Isotope	ND
U234_7	3.4793E-09	PU2407	1.7538E-04	AM2437	1.8887E-08
U235_7	3.2881E-06	PU2417	1.1644E-05	CM2427	1.8887E-08
U236_7	5.7531E-07	PU2427	2.8768E-06	CM2437	3.0378E-10
U238_7	4.5364E-04	AM2417	1.5283E-05	CM2447	1.8555E-09
NP2377	1.0493E-06	AM42M7	1.3676E-08	CM2457	6.7008E-11
PU2387	7.6205E-07	AM2427	2.5361E-08	CM2467	8.0760E-13
PU2397	5.1756E-04				

Table 3-4. Fuel Compositions of the 1D Test Problems 3 and 4

Case	Fuel Region		Non-Fuel Region	
	Isotope	ND	Isotope	ND
1D Case 3	U-235	2.0E-3	O-16	3.5E-03
	U-238	7.5E-3		
1D Case 4	U-235	2.0E-3	Fe-56	1.9486E-02
	U-238	7.5E-3	Na-23	3.4976E-03

Table 3-5 lists the comparison of eigenvalues produced from DIF3D and MCNP. Note that 230 group cross sections were used for the DIF3D calculations. As shown in the table, the eigenvalues estimated from DIF3D were in good agreement with the MCNP solutions within 90 pcm, except for the 1D problem case D which includes Fe-56 and Na-23 in the non-fuel region. The difference of 259 pcm is not too bad, but a further investigation may be necessary to find a main source of the error. Even though not listed in the table, the eigenvalues from DIF3D with 33-group cross sections without TWODANT calculations were still in good agreement with MCNP, but as noted previously, errors in neutron flux and power distributions were found to be much larger than those from the 230 group calculations specially in the non-fuel regions and around.

Table 3-5. Eigenvalues of DIF3D and MCNP for 2D and 1D Test Problems

Case	MCNP	DIF3D	Δk , pcm
2D Case 1	1.20773 $\pm$ 0.00007	1.20775	2
2D Case 2	1.12524 $\pm$ 0.00008	1.12449	-75
1D Case 1	1.14077 $\pm$ 0.00009	1.14129	52
1D Case 2	1.18847 $\pm$ 0.00009	1.18826	-21
1D Case 3	1.48919 $\pm$ 0.00012	1.49007	88
1D Case 4	1.49400 $\pm$ 0.00012	1.49141	-259

Figure 3-9 shows power distributions produced from neutron and gamma for the 2D problem case 1. As expected, the contribution to power is dominant by neutrons in the fuel regions and by gammas in the non-fuel regions. This is not the case for the control rod and shield regions because the (n, α) reaction is great due to the large amount of B-10. This can be proved in the 1D problem case 2, in which boron and carbon were removed from the 1D problem case 1, where the gamma contribution to power is dominant.

Total, neutron, and gamma power distributions for the 2D problem case 1 were compared as shown in Figure 3-10 and Figure 3-11 which show the DIF3D results with the 33-group neutron and 21-group gamma cross sections (the 21-group gamma library), the 230-group neutron and 21-group gamma cross sections (the 21-group gamma library), and the 230-group neutron and 94-group gamma cross sections (the 94-group gamma library), respectively. The total powers (i.e., the sum of neutron and gamma powers) of DIF3D and MCNP are normalized to be the same. Note that in the case with the 94-group gamma cross sections, the 94-group gamma calculation

were directly performed in DIF3D/GAMSOR. We tried to use the 94-group gamma library in MC²-3 in order to produce the 21-group gamma data which were used in DIF3D/GAMSOR, noting that it did not make differences from the use of the 21-group gamma library unless the TWODANT calculation was performed and then the resulting 94-group gamma fluxes were used for condensing the 94-group gamma data to the 21-group ones.

As can be seen in the figures that compare powers, the DIF3D neutron and gamma powers with the 33-group neutron and 21-group gamma cross sections showed larger than 15% errors compared to the MCNP solutions. Those errors were greatly reduced to less than 5% by using the 230-group neutron and 94-group gamma cross sections. This indicates that the two-step approach using the TWODANT calculation is required for both neutron and gamma calculations when using the 33-group neutron and 21-group gamma cross sections in DIF3D/GAMSOR.

Figure 3-12 shows the comparison of the total, neutron, and gamma power distributions between DIF3D and MCNP for the 2D test problem case 2 which contains plutonium fuel. There are no noticeable differences, in terms of magnitude and trend, from the comparison results obtained from the 2D test problem case 1. Since the DIF3D calculation was carried out using the 230-group neutron and 21-group gamma cross sections, the large differences of the gamma powers between the two codes would be greatly reduced when using the 94-group gamma cross sections, as indicated in the 2D test problem case 1. This indicates that the heating values of plutonium isotopes and high actinides from the new gamma library are reasonable.

For verification tests with more clean condition, 1D test problems were made with the same compositions used for the 2D problems and with simplified regions and compositions: i.e., 3 regions with no more than 2 isotopes for each region. Figure 3-13 shows the power distributions and comparison between DIF3D and MCNP. The comparison results are basically similar to the 2D problem case 1 since both use the same composition at least for the tallied regions. As noted previously, the large difference of the gamma power in the shield regions will be reduced if using the 94-group gamma cross sections. Interestingly, for the 1D problem case 2 where boron and carbon were removed from case 1, we observed a large difference of up to 17% in the neutron power even though the magnitude of the neutron produced power is very small and most of the power in the non-fuel region (80-100 cm) is produced by gamma. A follow-up investigation revealed that the difference came from sodium, indicating that the neutron heating factor would be overestimated for the isotope. Further investigation is needed for this problem.

Figure 3-14 and Figure 3-15 show the comparison of the neutron and gamma flux distributions over energy, respectively, between DIF3D and MCNP for the regions starting 60 cm (outer core) to the end (shield) where flux transition would be severe due to the change of material. As shown in the figures, the neutron and gamma fluxes between the two codes are overall in good agreement except for the low-energy range and the shield region approaching to the vacuum boundary condition, where the uncertainties of the MCNP solutions are relatively large as well. Note that for the comparison we used the DIF3D solutions based on the 33-group neutron and 21-group gamma cross sections (relatively low accuracy) and therefore the DIF3D solutions would be in better agreement, as shown in the power comparison, if they are updated with the 230-group neutron and 94-group gamma cross section results.

Figure 3-16 shows the power comparisons for the 1D problem 2 which is the same as the 1D problem 1 but sodium and carbon were removed from the control rod and shield regions. Because of no boron, the power produced from gamma are dominant at those regions and the relatively

large error in the neutron power estimation in the control rod region was observed, but the impact is very small because of very small power produced by neutrons. Note that the large error was caused by sodium as can be observed again in Figure 3-18.

The 1D test problems 3 and 4 would give more clear insights about how accurate the neutron and gamma calculation of MC²-3/DIF3D/GAMSOR is, since they use simplified regions and isotopes which would reduce error cancellation between isotopes and regions. Especially, the 1D test problem 3 is the simplest, having U-235 and U-238 (~20 w/o U-235 enriched fuel) in the fuel region and O-16 only in the non-fuel region. As can be seen in Figure 3-17, all powers agreed well with between DIF3D and MCNP, showing that the power produced by gamma from DIF3D is underestimated by 2%, compared to MCNP.

In the 1D test problem 4, as shown in Figure 3-18, the power produced by gamma from DIF3D is underestimated by up to 4%, compared to MCNP, and the large overestimation of power produced by neutron was observed in the non-fuel region, as observed in the 1D test problem 2. As discussed, it is caused by sodium but the contribution of neutron heating to the total power in the non-fuel region is very small.

To summary, the verification test results indicated that the total, neutron, and gamma powers generated from MC²-3/DIF3D/GAMSOR agreed well with the MCNP solutions when using the 230-group neutron cross sections and 94-group gamma data. For core calculations with 33-group neutron cross sections, we have used the two-step approach with MC2-3/TWODANT. Similarly, a gamma transport calculation with TWODANT using 94-group gamma cross sections may be necessary to condense the 94-group to 21-group gamma data in order to accurately obtain gamma fluxes in the non-fuel regions. Without the gamma transport calculation with TWODANT or the direct use of the 94-group gamma data, little or no improvements in accuracy were observed by using the 94-group gamma library.

Figure 3-9. Comparison of Total, Neutron and Gamma Powers between DIF3D (33G Neutron Cross Sections) and MCNP for the 2D Problem Case 1 (6 Regions)

Figure 3-10. Comparison of Total, Neutron and Gamma Powers from DIF3D (230G Neutron, 21G Gamma Cross Sections) for the 2D Problem Case 1 (6 Regions)

Figure 3-11. Comparison of Total, Neutron and Gamma Powers from DIF3D (230G Neutron, 94G Gamma Cross Sections) for the 2D Problem Case 1 (6 Regions)

Figure 3-12. Comparison of Total, Neutron and Gamma Powers between DIF3D (33G Neutron Cross Sections) and MCNP for the 2D Problem Case 2 (6 Regions)

Figure 3-13. Comparison of Total, Neutron and Gamma Powers between DIF3D and MCNP for the 1D Problem 1 (6 Regions)

Figure 3-14. Comparison of Regionwise 33G Neutron Fluxes between DIF3D and MCNP for the 1D Problem 1 (6 Regions)

Figure 3-15. Comparison of Regionwise 21G Gamma Fluxes between DIF3D and MCNP for the 1D Problem 1 (6 Regions)

Figure 3-16. Comparison of Total, Neutron and Gamma Powers between DIF3D and MCNP for the 1D Problem 2 (6 Regions)

Figure 3-17. Comparison of Total, Neutron and Gamma Powers between DIF3D and MCNP for the 1D Problem 3 (3 Regions)

Figure 3-18. Comparison of Total, Neutron and Gamma Powers between DIF3D and MCNP for the 1D Problem 4 (3 Regions)

3.3 EBR-II Benchmark Problems

The coupled neutron and gamma heating calculations were performed for the EBR-II benchmark problem [3] using DIF3D with the neutron and gamma cross sections and heating data generated from MC²-3. The EBR-II benchmark problem was constructed based on the core configuration of Run 138B, consisting of 71 regular driver fuel assemblies, 13 half-worth fuel driver assemblies, 10 control and safety assemblies, 6 structural assemblies, and 6 instrumented assemblies. These subassemblies contained 91 fuel pins. The half worth drivers also contained 91 pins, only 46 of which were fuel pins. The core is illustrated in Figure 3-19. The detailed core specifications can be found in References 2 and 16.

For the verification tests, the following old and new gamma libraries were used, all of which were generated using the ENDF/B-VII.0 data.

- 1) The old gamma library that was initially generated before 2016,
- 2) The current gamma library that was updated in 2016,
- 3) The new gamma library that was generated recently, including the delayed gamma and beta data.

The old gamma library was included in the test to reproduce the results obtained from the initial verification [3]. The new gamma libraries on the 21-group structure were used for the test, instead of the one with the 94-group structure. As discussed in the previous section, a gamma transport calculation with TWODANT should be done in order to obtain a noticeable improvement in accuracy by using the 94-group gamma library.

All of the three gamma libraries were constructed based on the 2,082 neutron group and 21 gamma group structures. For the simulation of the EBR-II core, the 33-group neutron cross section data were generated with MC²-3 using the two step approach, while the gamma cross sections (GAMISO) and production and heating data (PMATRX) were produced from MC²-3 based on the 33-group neutron and 21-group gamma structures.

The core calculations with DIF3D/GAMSOR were performed to solve the neutron and gamma transport equations using P5P3: a transport approximation of P₅ and an anisotropic scattering approximation of P₃. For comparison, a MCNP6 calculation was performed, tallying both neutron and gamma particles. The delayed fission gammas and delayed betas were not considered in both MC²-3/DIF3D and MCNP6 calculations for a consistent comparison.

Figure 3-20 shows % differences of assembly powers between MCNP and DIF3D with the old 21-group gamma library, confirming that it reproduced the results that we reported as an initial verification of the gamma produced powers [3] and showing that both DIF3D and MCNP results were in good agreement within 4.9%. The largest error occurred at the dummy fuel assembly as shown in the figure.

Figure 3-19. EBR-II Core Loading Pattern for Run 138B

Figure 3-20. Relative difference (%) of Assembly Powers between MCNP6 and MC²-3/DIF3D
Using the Old 21-group Gamma Library

Figure 3-21. Relative difference (%) of assembly powers between MCNP6 and MC²-3/DIF3D
Using the Current 21-group Gamma Library

Figure 3-22. Relative Difference (%) of Assembly Powers between MCNP6 and MC²-3/DIF3D
Using the New 21-group Gamma Library

Figure 3-23. Relative Difference (%) of Assembly Powers between MCNP6 and MC²-3/DIF3D Using the New 91-group Gamma Library

$$< \% \text{ Difference} = [P(\text{w/ Delayed}) - P(\text{w/o Delayed})] / P(\text{w/o Delayed}) * 100 >$$

Figure 3-24. Relative Difference (%) of Assembly Powers between Two MC²-3/DIF3D Results Using the New 21-group Gamma Library with and without Delayed Gamma and Betas

Figure 3-21 gives % differences of assembly powers between MCNP and DIF3D with the current 21-group gamma library (maximum 3.1%), showing some improvements in power estimation compared to the result with the old 21-group gamma library (maximum 5%). While the results with the old gamma library underestimated powers at the dummy fuel assemblies, those with the current gamma library slightly overestimated powers at those regions.

Figure 3-22 and Figure 3-23 show % differences of assembly powers between MCNP and DIF3D with the new 21-group gamma library and the new 94-group gamma library, respectively. As mentioned previously, the group condensation of gamma data from 94 to 21 groups were made using the gamma spectrum produced from a homogeneous composition based gamma transport calculation (i.e., no TWODANT calculation was performed). Interestingly, the maximum % difference was reduced to 1.5% for the case using the new 21-group gamma library, but it rather increased to 4.1% for the case using the new 94-group gamma library.

The new 21-group gamma library with the delayed gamma and betas was used to simulate the EBR-II problem. The DIF3D results with and without the contributions of the delayed gamma and betas were compared, showing the power increase by up to 26% at all dummy assemblies and part of the experiment assemblies, as seen in Figure 3-24. The similar trend in power change was observed in MCNP calculations with and without the delayed gamma and beta contributions [8].

4. Conclusions

The new gamma library was generated based on the 94-group gamma structure, including delayed gamma and beta data, using the PreGAMMA and GenGAMMA codes with ENDF/B-VII.0 data. In order to verify the new gamma library, the 2D benchmark problems that were introduced in the GAMSOR manual were solved and inspected. Additionally, simpler 1D problems with different material configurations were developed to support verification tests. Finally, the EBR-II benchmark problem was solved again and compared with the solutions with the previous gamma libraries as well as MCNP solutions.

Unlike the noticeable errors reported in the GAMSOR manual, it was found from the 2D benchmark problem that the neutron and gamma heatings were in good agreement with MCNP solutions within 5% even in the non-fuel regions of both cores with uranium or plutonium dominant fuel compositions. In the simpler 1D problems with 3 or 6 regions, similarly, we observed good agreement in neutron and gamma powers between DIF3D and MCNP. Note that the 230-group neutron and 94-group gamma data were used in all the MC2-3/DIF3D/GAMSOR calculations. It indicates that the group collapsing should be made properly using TWODANT RZ solutions if 33-group neutron and 21-group gamma data are used, in order to maintain such a good accuracy.

The calculations of the EBR-II benchmark problem showed that the DIF3D solution with the new gamma library maintained good agreement in the power distribution with the MCNP solution. Interestingly, the differences in the power distribution were reduced further when using the new 21-group gamma library, compared to the DIF3D results with the new 94-group gamma library. With the inclusion of delayed gamma and beta data, the powers in the dummy assemblies were increased by up to 26%, which could not be verified with MCNP solutions explicitly but should be correct in terms of the direction of change.

Overall, the verification results indicate that the new gamma library were generated correctly, providing reasonable solutions for all the benchmark problems that were solved in this study. However, further detailed verification tests may be necessary and, more importantly, validation tests are required against measurement data.

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